

Non-Gaussian distribution of collective operators in quantum spin chains

M. Moreno-Cardoner,¹ J. F. Sherson,² and G. De Chiara¹

¹*Centre for Theoretical Atomic, Molecular and Optical Physics Queen's University, Belfast BT7 1NN, United Kingdom*

²*Department of Physics and Astronomy, Ny Munkegade 120, Aarhus University, 8000 Aarhus C, Denmark*

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We numerically analyse the behavior of the full distribution of collective observables in quantum spin chains. While most of previous studies of quantum critical phenomena are limited to the first moments, here we demonstrate how quantum fluctuations at criticality lead to highly non-Gaussian distributions thus violating the central limit theorem. Interestingly, we show that the distributions for different system sizes collapse after scaling on the same curve for a wide range of transitions: first and second order quantum transitions and transitions of the Berezinskii-Kosterlitz-Thouless type. We propose and carefully analyse the feasibility of an experimental reconstruction of the distribution using light-matter interfaces for atoms in optical lattices or in optical resonators.

Introduction.- The understanding of phase transitions and critical phenomena lies at the very heart of condensed-matter physics [1]. Standard quantum phase transitions, i.e. those following Landau's theory, are signalled by the onset of a local order parameter when local symmetries are broken [2]. This theory sets the mean value of the order parameter at the center of stage. However, going beyond the first order moment reveals interesting information about the many-body state without performing a full state tomography. For instance, in experiments with ultracold atoms, noise correlations reveal antiferromagnetic ordering [3, 4]; variances of collective operators in the form of structure factors allow one to distinguish between quantum phases such as the superfluid and Mott insulator [5], and to detect antiferromagnetic or crystal ordering [6] and collective entanglement [7, 8]; the kurtosis, related to higher order moments, provides information about quasiparticle dynamics and their interactions [9]; and the full distribution of contrast in interference experiments can reveal strongly correlated atomic states [10].

In this paper we go beyond the first moments of the order parameter and analyse the full probability distribution function (PDF) of collective operators in spin chains. The PDF of the order parameter plays a central role in statistical mechanics. When the correlation length is finite, deep in an ordered phase, the system can be regarded as the sum of independent subblocks of finite length and the central limit theorem leads to a Gaussian PDF, in agreement with the Landau paradigm. Instead, at criticality, the divergence of the correlation length leads to a non-trivial highly non-Gaussian function, which characterizes the transition. Moreover, if hyperscaling relations hold [13, 14], the function is universal and shows scaling behavior.

The PDF of the magnetization has been exhaustively studied in classical spin systems undergoing phase transitions [15–21]. However, much less attention has been paid to its quantum counterpart [22, 23]. Non-Gaussian distributions of light fluctuations have been observed for cold atomic ensembles [24]. Nevertheless, a systematic treat-

ment in the case of strongly-correlated atoms is currently missing. In this context, quantum coherent fluctuations of the individual constituents can lead to non-Gaussian PDFs, which are a necessary resource for continuous variables quantum information processing [25]. Furthermore, all statistical moments, related to many-body correlation functions, can be extracted from this function. The PDF thus contains non-local information of the system, and it can be connected to non-local order parameters in certain quantum phases. Using exact solutions and the density matrix renormalisation group (DMRG) [26], we analyze the PDF of collective spin variables for different types of quantum phase transitions (first, second and BKT type), paying special attention to their behavior at criticality. Furthermore, we give an example of how this can be connected to a non-local order parameter. Finally, we propose two possible experimental setups based on optical lattices for the measurement of the PDF, the first employing high resolution microscopy and the second quantum polarization spectroscopy.

Probability density functions.- The probability to observe an eigenvalue m of an operator M is given by $P(m) = \sum_{\mu} \langle m_{\mu} | \rho | m_{\mu} \rangle$, where ρ is the density matrix describing the system and $\{|m_{\mu}\rangle\}$ an orthonormal set of eigenstates of M compatible with m . If M is the order parameter, one can establish a direct relation with the free energy functional $\mathcal{F}[m]$ appearing in Landau formalism [2]: $P(m) \sim e^{-\mathcal{F}[m]}$. $\mathcal{F}[m]$ can be approximated by a power series of m and, if quantum correlations do not diverge, the lowest order terms dominate. This leads to a PDF which is approximately Gaussian, a result which can also be understood by the central limit theorem. In contrast, close to the critical point we expect a highly non-Gaussian PDF.

Finite size scaling.- Close to a continuous (second order) transition induced by a parameter g of the Hamiltonian with critical point g_c , the correlation length diverges as $\xi \propto \tau^{-\nu}$, where $\tau = |g - g_c|$ and ν is the critical exponent. Close enough to the critical point, the finite size scaling hypothesis implies that the mean value $\langle M \rangle$ scales

with the system size L as [28]:

$$\langle M \rangle = L^{-\beta/\nu} f(\tau L^{1/\nu}) \quad (1)$$

where f is an analytic function. It is often more convenient and accurate for determining the critical point, both numerically and experimentally, to compute the Binder cumulant: $U = 1 - \langle M^4 \rangle / 3 \langle M^2 \rangle^2$, as its scaling depends only on ν and not on β . That is, $U = \tilde{f}(\tau L^{1/\nu})$, with a different scaling function \tilde{f} . U quantifies the Gaussianity of the PDF, being null for a Gaussian distribution centered at zero.

Here we go beyond the first moments and consider the full probability distribution function $P_L(m, g)$. The renormalised PDF is expected to be a universal function:

$$\tilde{P}(\tilde{m}, r) = L^{-\beta/\nu} P_L(m, g) \quad (2)$$

with $\tilde{m} = m/L^{-\beta/\nu}$ and $r = L/\xi$. This implies hyperscaling and finite-size scaling of higher order correlation functions hold [15, 16, 20]. In fact, when the actual critical exponents are unknown, one can instead rescale these quantities with the scale $\sigma = \sqrt{\langle (M_x^{st})^2 \rangle}$, directly computed from the PDF.

Models and Methods.- We consider a variety of spin-1/2 chain models encapsulated by the Hamiltonian:

$$H = \sum_{i,\alpha} (J_\alpha \sigma_\alpha^i \sigma_{\alpha+1}^i + h_\alpha \sigma_\alpha^i) \quad (3)$$

where the sum on i extends over the L spins in the chain. The Pauli operators of spin i are denoted by σ_α^i , while J_α and h_α are coupling constants and magnetic fields along different directions ($\alpha = x, y, z$). This model exhibits various transitions [1, 11, 12], some of which will be discussed below. We will study the behaviour of collective operators such as the total magnetization $M_\alpha = \sum_i \sigma_\alpha^i / L$ and its staggered counterpart $M_\alpha^{st} = \sum_i (-1)^i \sigma_\alpha^i / L$.

Analytical results for the PDF can be obtained for models that can be written with a free fermionic representation after the Jordan-Wigner transformation, i.e. $J_z = h_{x,y} = 0$ in Eq.(3) assuming periodic boundary conditions, and operators that are separable in this basis, as for example M_z . The order parameter M_x however, is not separable and contains the string order operator. In principle all its powers could be computed by means of Wick's theorem, but the evaluation becomes involved as the order increases. At criticality, the PDF can be exactly obtained by exploiting the relation with Kondo physics [23], but reconstructing the PDF becomes in general a very challenging task. Here instead, to obtain the PDF, we combine two different numerical methods. We use exact diagonalisation for sizes up to 20 sites, and also the time-dependent density matrix renormalisation group [26] with open boundary conditions. Using the latter, the PDF can be evaluated from the characteristic function, related to P_L by a discrete Fourier transform.

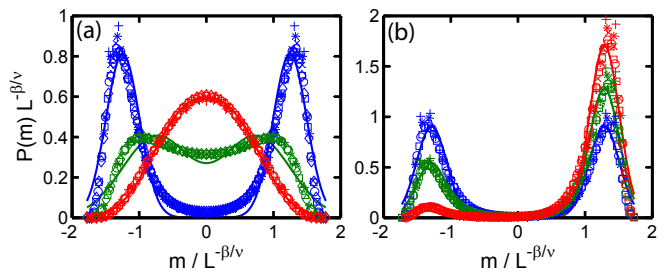


FIG. 1: (Color online) Rescaled PDF of the order parameter in the transverse Ising model. Data collapse is observed for different system sizes (from $L = 20$ to $L = 100$), denoted by different symbols. (a) In absence of longitudinal field and for different phases at fixed r : FM ($r = 4$, blue), critical ($r = 0$, green) and PM ($r = 4$, red). (b) In presence of the longitudinal field in the FM phase ($r = 4.8$) and $q = 0$ (blue), $q = 0.5$ (green) and $q = 2$ (red). The PDF is non-Gaussian close to the critical point.

Second order transition.- We set $J_{y,z} = h_{x,y} = 0$, $J_x = J < 0$ and $h_z = Jg$ in Eq.(3), corresponding to the ferromagnetic transverse Ising model, which exhibits a second order phase transition at $g = \pm 1$ separating a ferromagnetic ordered phase (FM) at low fields and a paramagnetic disordered phase (PM) at high fields. In Fig. 4(a) we show the numerical results for the PDF of the spontaneous magnetization M_x , the order parameter in FM. Remarkably, we have obtained data collapse already for relatively small system sizes, assuming the ansatz of Eq.(2) with the predicted values $\beta = 1/8$ and $\nu = 1$ (see e.g. [13, 14]). This result reinforces the scaling hypothesis of all the statistical moments of the order parameter. Away from the critical point and in the thermodynamic limit ($r \rightarrow \pm\infty$) the PDF is Gaussian, in agreement with Landau theory and the central limit theorem. In the disordered phase, it is centered around $m = 0$, whereas in the ordered phase the distribution is bimodal with the two peaks corresponding approximately to the broken-symmetry values of the order parameter. We have quantified the Gaussianity of the distribution by fitting the data with the sum of two Gaussians (see solid lines in Fig. 4(a)), and find very good agreement away from the critical point. In contrast, at criticality ($r \rightarrow 0$) the fitting yields poor results and one should instead use the exponential of a higher-order polynomial. The central limit theorem does not hold anymore due to quasi long-range fluctuations in this regime. The norm of the residuals signals very clearly the critical point, with a sudden increase around its value, as shown in the Supplementary Material [48]. There we also report data collapse for the Binder cumulant U . Finally, for comparison, we note that for an observable which is not the order parameter, such as M_z , the PDF is always Gaussian.

First order transition.- We consider the same Hamiltonian as before but with an additional longitudinal field $h_x = Jh \neq 0$. At fixed value of the transverse field

$g = \pm 1$ and approaching the Ising critical point by varying only h , the quantum phase transition is characterized by a different set of exponents ($\beta = 1/15$ and $\nu = 8/15$ [13]). Our results (not shown) support strong evidence of scaling of the PDF.

If instead, the longitudinal field h is varied across zero, but at fixed value of the transverse field $|g| < 1$, the system undergoes a first order transition between two ferromagnetic states with opposite magnetization M_x . At this transition, neither the correlation length diverges nor the gap closes. Nevertheless, inspired by Ref. [27], we propose a finite size scaling of the PDF.

In a finite size chain, two different energy gaps are present in this model. One is the real energy gap in the thermodynamic limit, which at $h = 0$ is given by $\Delta E = ||g| - 1|^{\nu/z}$ with $z = 1$, and it closes at the Ising critical point ($g = \pm 1$). The other gap δ separates the two lowest eigenstates and it is minimum at $h = 0$, with value $\delta_0 = 2|J|(1 - g^2)g^L$, decreasing exponentially with L ($|g| < 1$). In [27], following dimensional arguments, the authors assume that δ and M_x only depend on the longitudinal field h and L through the ratio q between the two energy scales: the first associated with the longitudinal field $hLM_{x,0}$, being $M_{x,0} = (1 - g^2)^{1/8}$ the magnetization at $h = 0$, and the second δ_0 :

$$q = \frac{2hLM_{x,0}}{\delta_0} = \frac{hL}{(1 - g^2)^{7/8}g^L}. \quad (4)$$

Thus, $\delta \sim \delta_0(g)f_1(q)$ and $M_x \sim m_0(g)f_2(q)$, where $f_{1,2}(q)$ are analytic functions at $q = 0$.

Here, we conjecture a similar dependency for the correlation length: $\xi \sim \xi_0(g)f(q)$ where f is analytic at $q = 0$, and $\xi_0(g) = \xi(q = 0, g)$ diverges close to the Ising critical point with the usual power law: $\xi_0(g) \sim ||g| - 1|^{-\nu}$. Moreover, any observable $M_L(g, h)$ depends only on the ratios $r = L/\xi_0$ and q when rescaled with the proper critical exponents, e.g. for the magnetization $\bar{M}_x(r, q) = L^{-\beta/\nu}M_{x,L}(g, h)$. Indeed, at fixed values of r and q , we observe again data collapse for the PDF for different lengths, as shown in Fig. 4(b). We find the distribution to be always bimodal with the relative height of the two peaks ruled by h_x . We fitted the data with the sum of two Gaussians and found reasonable agreement except at the critical point, due to non-linear effects in the Landau potential.

BKT transition. - For completeness, we finish this analysis with a different type of transition, the Berezinski-Kosterlitz-Thouless (BKT) transition in the spin-1/2 XXZ model. We set $h_{x,y,z} = 0$, $J_{x,y} = J > 0$ and $J_z = J\Delta$ in Hamiltonian (3). The phase diagram is well known: the ground state is ferromagnetic for $\Delta < -1$, critical for $|\Delta| < 1$, and with Néel order for $\Delta > 1$. The BKT transition is at $\Delta = 1$. We compute the PDF for the staggered magnetizations $M_{x,z}^{st}$. In this case, we rescale the quantities m and $P(m)$ with σ as defined before. For M_z^{st} , which corresponds to the order parameter in the

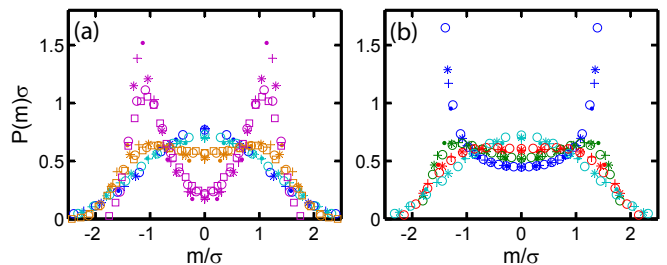


FIG. 2: (Color online) Rescaled PDF in the spin-1/2 XXZ model. Data collapse is observed for different system sizes (from $L = 10$ to $L = 60$), denoted by different symbols. (a) For J_z^{st} at fixed r : critical ($r = 0.9, 0$; blue and cyan), Néel order ($r = 0.35, 1.3$; orange and purple). (b) For J_x^{st} at fixed Δ : critical ($\Delta = -0.99, -0.5, 0, 1$; blue, green, red and cyan).

Néel phase, we also fix $r = L/\xi$, being $\xi = e^{\pi/\sqrt{|\Delta|-1}}$ [12], and observe data collapse for different system sizes, as shown in Fig. 5(a). As expected, the distribution tends in the thermodynamic limit to a double- and single-peaked Gaussian for $\Delta > 1$ and $\Delta < 1$, respectively.

As shown in Fig. 5(b), the situation is much more interesting for the PDF of M_x^{st} , for which the spin-spin correlations do not decay exponentially in the critical phase ($|\Delta| < 1$). Outside this interval the distribution is Gaussian and centered at zero, because the operator M_x^{st} is disordered, while in the critical phase it is highly non-Gaussian. We observe again data collapse for different chain lengths, but now by fixing the value of Δ . The scaling with fixed Δ is expected to occur in a critical phase, where the energy gap has already closed. When crossing the first order transition at $\Delta = -1$, the PDF shows a discontinuity, with a sudden jump from a Gaussian to a singular function that diverges at the edges. Across the critical phase, the function changes continuously from a double-peak structure for $\Delta < 0$ to a single peak distribution for $\Delta > 0$. At the BKT point the PDF tends again to a Gaussian in the thermodynamic limit. Note that the results for the ferromagnetic model $J < 0$ are equivalent when analyzing M_x instead, and changing $\Delta \leftrightarrow -\Delta$. The non-Gaussianity in the critical phase is also evident from the analysis of the Binder cumulant reported in the Supplementary Material [48].

Non-local order parameters. - The BKT transition is particularly relevant in the context of 1D optical lattice gases because it rules the superfluid (SF) to Mott insulator (MI) transition in the Bose-Hubbard model. Close to the MI, where density fluctuations are small, and for large enough integer fillings, the model can be approximated to an effective spin-1 model [29, 30]. The SF and MI are mapped respectively to the critical ferromagnetic phase, and to a state with local magnetization $S_z^i = 0$ perturbed with tightly bound particle-hole fluctuations. The nature of density fluctuations is however different in the two phases. In the MI the non-local correlations can

be characterized by the parity operator defined as

$$\mathcal{O}_P^2 = \lim_{l \rightarrow \infty} \left\langle \prod_{k \leq j \leq k+l} e^{i\pi \delta n_j} \right\rangle \quad (5)$$

where δn_j is the local excess density from the average filling [31–33], and corresponds to the local magnetization in the magnetic model. \mathcal{O}_P^2 is finite in the MI, while it vanishes in the SF, and it has been experimentally reconstructed in [33] using single site microscopy.

In this context, an additional motivation for the study of PDFs is that it captures these non-local correlations. Indeed, it is easy to see that the characteristic function $X(u) = \sum_m e^{i u m} P(m)$ for the suitable collective variable (in this case, the average magnetization of a subblock of length l) at frequency $u = l\pi$ is equal to the parity operator $\lim_{l \rightarrow \infty} X(u = l\pi) = \mathcal{O}_P^2$. Thus, a measurement of a collective variable and the reconstruction of its PDF provides an alternative route to evaluate non-local order parameters besides lattice modulation spectroscopy [31].

Experimental reconstruction of the PDF.— The PDF for the local number parity operator can be reconstructed using single site resolution microscopy [34, 36]. Recently, novel schemes which allow to circumvent light-assisted pair loss and resolve the internal atomic degree of freedom have been also demonstrated [35]. An alternative proposal is based on the Faraday effect, and consists in analysing the polarization fluctuations of a strongly polarised laser beam that interacts with the atomic sample [37–39]. Since this is based on dispersive light-matter interaction, it has the advantage of being less destructive, which could potentially pave the way for multiple probing of the same ensemble. Furthermore, this scheme could be exploited as in [40] for the conversion of atomic correlations and entanglement into the light degree of freedom for quantum information processing. The light-matter interaction with the collective spin operator M , $H_{\text{eff}} \sim (\tilde{\kappa}/\tau) L P_{ph} M$, is written in terms of the momentum-like light quadrature P_{ph} measuring the photon fluctuations in the circular basis with respect to the strong polarisation axis, and τ is the interaction time. P_{ph} is canonically conjugated to its position-like counterpart: $[X_{ph}, P_{ph}] = i\hbar$. The coupling constant $\kappa = (\eta\alpha)^{1/2}$ can be expressed in terms of the single atom excitation probability or destructivity η , and the resonant optical depth $\alpha = N\sigma_{\text{cross}}/A$, where A is the overlap area between light and atoms, σ_{cross} is the resonant cross section and for a one-dimensional system $N = L$. By adjusting the laser intensity, the destructivity parameter η is typically set to values smaller than 0.1 to limit the fraction of excited atoms. The resonant optical depth α should be maximized in order to obtain the largest possible coupling between light and atoms. For ultracold atoms in a one-dimensional optical lattice, considering $L = 100$ and $A = 0.5\mu\text{m}^2$ we obtain $\alpha \approx 8$ and $\kappa \approx 1$. We define $\tilde{\kappa} = \kappa/\sqrt{L}$, which will be approximately inde-

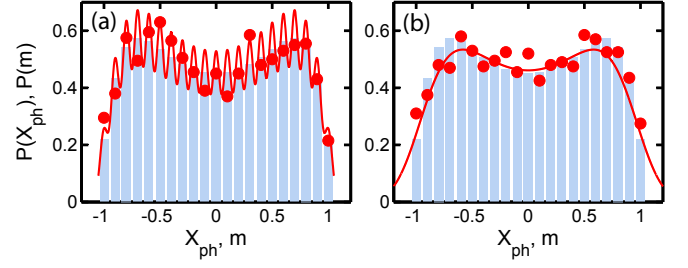


FIG. 3: (Color online) Comparison between rescaled light distribution (red solid line) and PDF of the order parameter (blue bar) in the critical phase in the Transverse Ising model for (a) $\tilde{\kappa} = 1.0$, $\sigma_{ph}^2 = 1/2$ and (b) $\tilde{\kappa} = 0.15$, $\sigma_{ph}^2 = 1/4$. The red circles correspond to the histogram obtained with a random variable following the light distribution for a number of shots $N_{sh} = 2000$.

pendent of L and can be as large as $\tilde{\kappa} \sim 0.1$. We will show that this value of κ is large enough to reconstruct the PDF of the spin operator M by looking at the distribution of the light quadrature X_{ph} . Larger values of $\tilde{\kappa}$ could be engineered by coupling atoms with optical cavities [41, 42], nanophotonic crystals [43, 44] or optical nanofibers [45].

It is possible to show [46] that the light distribution is the sum of vacuum Gaussian distributions of light each displaced by a quantity proportional to the eigenvalue m of the operator M and scaled by the probability $P(m)$ to observe such eigenvalue:

$$P(X_{ph}) = \sqrt{\frac{1}{2\pi\sigma_{ph}^2}} \sum_m P(m) e^{-(X + \tilde{\kappa} N m)^2 / (2\sigma_{ph}^2)} \quad (6)$$

where we have considered a Gaussian input light beam with variance σ_{ph}^2 , being $1/2$ for the vacuum state.

To evaluate the effectiveness of the method we compare the actual atomic spin distribution with the one of the output light. The distance between both distributions decreases exponentially with $\tilde{\kappa}/\sigma_{ph}$. Thus, one could in principle improve the fidelity by increasing $\tilde{\kappa}$ or using squeezed light [47]. We show in Figure 6 the result for the transverse field Ising model for an optimal case $\tilde{\kappa} = 1$ and $\sigma_{ph}^2 = 1/2$ and for a more realistic value of $\tilde{\kappa} = 0.15$, but squeezed input light with $\sigma_{ph}^2 = 1/4$, recently achieved [47]. For the former, the light distribution faithfully follows the magnetization, whereas for the later, it only agrees qualitatively, but still captures the peaks. Experimentally, one would need to repeat the measurement a number of shots $N_{shots} \sim L^2$ to estimate the PDF.

In conclusion, we have shown that the distribution of collective variables in spin models reveals relevant information of quantum phase transitions. We have shown that for a range of quantum phase transitions a non-Gaussian distribution of the order parameter is a clear signature of criticality, and that the scaling

hypothesis holds. Finally we have proposed an experimental method for its measurement using light-matter interfaces, and discussed its feasibility for realistic values.

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SUPPLEMENTARY MATERIAL

FITTING TO A GAUSSIAN DISTRIBUTION

We present here the results for the correlation coefficient corresponding to a non-linear least square fitting of the computed PDF in the transverse Ising model. We have fitted $P(m)$ to the function

$$P_{\text{fit}}(m) = \frac{1}{2\sqrt{2\pi\sigma^2}} \left[e^{-(m-m_0)^2/(2\sigma^2)} + e^{-(m+m_0)^2/(2\sigma^2)} \right] \quad (7)$$

with σ^2 and m_0 fitting parameters (see solid lines in Fig. 4(a) in the main file). The correlation coefficient is defined as:

$$c = \sqrt{1 - \delta y^2 / \text{Var}[y]} \quad (8)$$

where δy^2 is the squared norm of the residuals of the data y and $\text{Var}[y]$ the corresponding variance. This quantity is close to one when the fitting works well, whereas it drops to smaller values for a poor fitting. In Fig. 4 we show c as a function of the ratio $r = L/\xi \cdot \text{sgn}(h-1) = L(h-1)$, where ξ is the correlation length, for the transverse Ising model. It shows a sudden decrease close to the critical point, i.e. $r = 0$, and it tends to one away from the critical point, i.e. $r \rightarrow \pm\infty$.

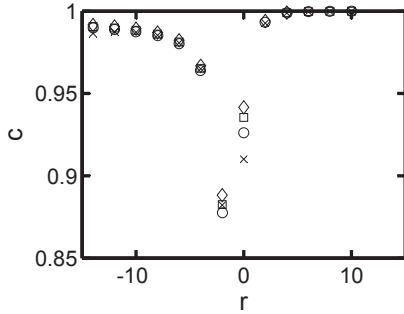


FIG. 4: Correlation coefficient c of a non-linear least square fitting of the PDF $P(m)$ to the function $P_{\text{fit}}(m)$ in the transverse Ising model. c suddenly decreases close to the critical point, indicating the PDF is non-Gaussian.

BINDER CUMULANT

Another possible way to quantify the Gaussianity of the PDF is by evaluating the Binder cumulant U , defined as

$$U = 1 - \langle M^4 \rangle / 3 \langle M^2 \rangle^2 \quad (9)$$

where M is the order parameter operator. U vanishes for a Gaussian distribution centered at zero, whereas it

tends to $U \rightarrow 2/3$ for a distribution close to two symmetric delta functions. Evaluating U is convenient for locating the critical point, since its finite size scaling only depends on the critical exponent ν and not on β . That is, $U = \tilde{f}(\tau L^{1/\nu})$, with a different scaling function \tilde{f} . Thus, when plotted as a function of the tuning parameter g , the crossing point for data corresponding to different sizes tends to the actual critical point. When instead, plotted as a function of $r = L/\xi$, they collapse to the same curve, which depends, however, on the boundary conditions.

In Fig. 5 we show the result of U for the Transverse Ising model with open boundary conditions (OBC) as a function of $r = L/\xi = L(h-1)$ (left) and h (right) for different system sizes, ranging from $L = 20$ to $L = 100$. In the left panel, the result for periodic boundary conditions (PBC) is also shown for comparison.

In Fig. 6 we show the result of U for the spin-1/2 XXZ model for the two observables M_z^{st} (left) and M_x^{st} (right), as a function of Δ . The Binder cumulant for M_z^{st} tends to the value $U \rightarrow 2/3$ in the Néel phase in the thermodynamical limit, whereas the one for M_x^{st} remains finite in the critical phase.

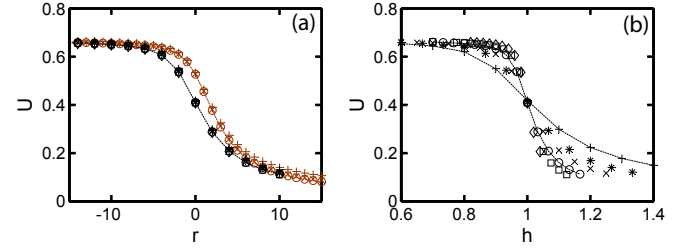


FIG. 5: (Color Online) Binder Cumulant U in the Transverse Ising model with OBC, for different system sizes denoted by different symbols (from $L = 20$ to $L = 100$). (a) As a function of $r = L/\xi \cdot \text{sgn}(h-1) = L(h-1)$, data collapse is observed. The brown symbols are for PBC. (b) As a function of h for OBC.

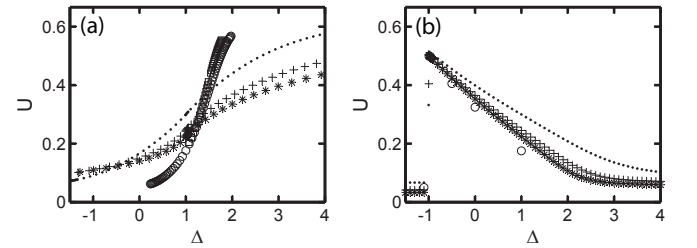


FIG. 6: Binder Cumulant U in the spin-1/2 XXZ model, for different system sizes denoted by different symbols (from $L = 10$ to $L = 60$). (a) For M_z^{st} it tends to $U = 2/3$ in the Néel ordered phase in the thermodynamic limit. (b) For M_x^{st} it remains finite in the critical phase in the thermodynamic limit.